

Spontaneous emissions and thermalization of cold bosons in optical lattices

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(Dated: May 8, 2013)

We study the thermalization of excitations generated by spontaneous emission events for cold bosons in an optical lattice. Computing the dynamics described by the many-body master equation, we characterize equilibration timescales in different parameter regimes. For simple observables, we find regimes in which the system relaxes rapidly to values in agreement with a thermal distribution, and others where thermalization does not occur on typical experimental timescales. Because spontaneous emissions lead effectively to a local quantum quench, this behavior is strongly dependent on the low-energy spectrum of the Hamiltonian, and undergoes a qualitative change at the Mott Insulator-superfluid transition point. These results have important implications for the understanding of thermalization after localized quenches in isolated quantum gases, as well as the characterization of heating in experiments.

PACS numbers: 37.10.Jk, 67.85.Hj, 03.75.Lm, 42.50.-p

Spontaneous emission is a fundamental source of heating in optical dipole potentials [1, 2], and one of the key heating sources in current experiments with cold atoms in optical lattices [3, 4]. This heating induces non-equilibrium dynamics in which thermalization processes are expected to play a key role. Typically it is assumed that the energy added to the system will be thermalized, causing an effective increase in temperature. But does that happen?

This question is a special case of a fundamental problem in many-body quantum mechanics: to what extent, and under which conditions, will an isolated system undergo thermalization when perturbed away from equilibrium, in the sense that at long times the system reaches a steady state where simple observables take the same values as those of a thermal distribution [5–8]. Recently, integrable dynamics for strongly interacting cold gases confined to move in 1D [9] has been observed, allowing the study of systems that either do not thermalize [10] or undergo generalized thermalization [11, 12].

In this Letter we investigate these issues by studying dynamics induced by spontaneous emission events (incoherent light scattering) for cold bosons in an optical lattice [13], and identify contrasting parameter regimes where (i) certain observables relax over short times to thermal values, or (ii) the system relaxes on a short timescale to states that are clearly non-thermal, even if all atoms remain in the lowest Bloch band. In particular, the dynamics depends greatly on the low-energy spectrum of the Hamiltonian because spontaneous emissions give rise to a local quench, leading to qualitative changes at the superfluid-Mott Insulator phase transition. By combining time-dependent density matrix renormalization group (t-DMRG) methods [14–17] with quantum trajectory techniques [18–20], we compute the dynamics

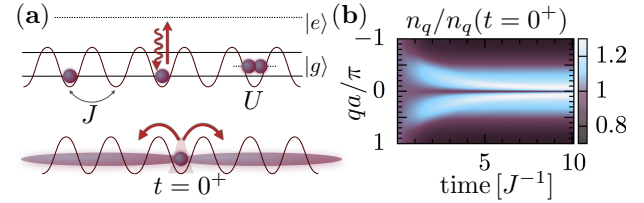


FIG. 1: (Color online) (a) Absorption and spontaneous emission of a lattice photon leads effectively to localization of single atoms. Tunnelling and interactions between atoms then redistribute the energy added to the system. (b) Localization of an atom in space corresponds initially to a distribution of the atom over the whole Brillouin zone (the tails of the quasi-momentum distribution are lifted). Subsequent unitary evolution leads to a broadened quasi-momentum distribution, *i.e.*, the $n_{q=0}$ peak and the tails decrease, while the small quasi-momentum components increase (t-DMRG results, $U = 2J$, $N = 48$ particles on $M = 48$ sites, $d_l = 6$, $D = 512$).

in the context of real experiments. These results have important implications for the characterization of heating in current experiments [21]. In fact, the lack of thermalization of certain excitations may be exploited to enhance the realization of fragile many-body states [22–25], leading to greater robustness of quantum simulators [26, 27].

In Ref. [4], a many-body master equation was derived to describe spontaneous emission processes for bosonic atoms. For far-detuned optical fields, we can adiabatically eliminate the excited atomic levels, obtaining an effective equation for ground-state atoms. When the lattice spacing a is comparable to or greater than the optical wavelength of scattered photons, $a \gtrsim \lambda$, the dynamics of the many-body density operator ρ is ($\hbar \equiv 1$), $\dot{\rho} = -i[H, \rho] + \mathcal{L}_1\rho$, where the dissipative term describing

scattering of laser photons, denoted $\mathcal{L}_1\rho$ is

$$\mathcal{L}_1\rho = -\frac{1}{2} \sum_{\mathbf{k}\mathbf{l}\mathbf{m}\mathbf{n}} \gamma_{\mathbf{k}\mathbf{l}\mathbf{m}\mathbf{n}} \left[b_{\mathbf{i}}^{(\mathbf{k})\dagger} b_{\mathbf{i}}^{(\mathbf{l})}, \left[b_{\mathbf{i}}^{(\mathbf{m})\dagger} b_{\mathbf{i}}^{(\mathbf{n})}, \rho \right] \right], \quad (1)$$

and H is a multi-band Bose-Hubbard Hamiltonian [4],

$$H = - \sum_{\mathbf{n}, \langle i, j \rangle} J^{(\mathbf{n})} b_{\mathbf{i}}^{(\mathbf{n})\dagger} b_{\mathbf{j}}^{(\mathbf{n})} + \sum_{\mathbf{n}, \mathbf{i}} \varepsilon_{\mathbf{i}}^{(\mathbf{n})} b_{\mathbf{i}}^{(\mathbf{n})\dagger} b_{\mathbf{i}}^{(\mathbf{n})} \quad (2)$$

$$+ \sum_{\mathbf{i}, \mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n}} \frac{1}{2} U^{(\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n})} b_{\mathbf{i}}^{(\mathbf{k})\dagger} b_{\mathbf{i}}^{(\mathbf{l})\dagger} b_{\mathbf{i}}^{(\mathbf{m})} b_{\mathbf{i}}^{(\mathbf{n})}. \quad (3)$$

Here, the 3D band indices are denoted by $\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n}$, and $b_{\mathbf{i}}^{(\mathbf{n})\dagger}$ is a bosonic creation operator for an atom on site \mathbf{i} in band \mathbf{n} . The dissipative dynamics involves scattering of photons and (in some cases) transitions between Bloch bands with the corresponding rates denoted $\gamma_{\mathbf{k}\mathbf{l}\mathbf{m}\mathbf{n}}$, while the tunnelling in band \mathbf{m} between neighboring sites $\langle i, j \rangle$ is denoted $J^{(\mathbf{n})}$, on-site interactions are denoted $U^{(\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n})}$ and an onsite potential $\varepsilon_{\mathbf{i}}^{(\mathbf{n})}$. Note that this includes the band energy $\omega^{(\mathbf{n})}$ as well as (potentially) an external trapping potential. The parameters can be calculated from the microscopic model by expanding in a basis of Wannier functions [4], though care must be taken to use properly regularized potentials in evaluating the interaction matrix elements $U^{(\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n})}$ [28–30].

In deep optical lattices, transition rates for *inter-band* processes coupling neighboring Bloch bands are suppressed by the square of the Lamb-Dicke parameter, $\eta = 2\pi a_T/\lambda$, where a_T is the trap length for the lowest band Wannier function. For typical experiments with lattice depths around $V_0 = 8E_R$ [with $E_R = 4\pi^2\hbar^2/(2m\lambda^2)$, where m is the mass of the atom], the suppression is $\eta^2 \sim 0.1$. In the usual case of a red-detuned optical lattice the dominant dissipative processes are thus *intra-band* processes, which return the atoms to their initial Bloch band. Processes accessing higher Bloch bands are suppressed by a factor of the order η^4 or greater, and we can write an effective two-band master equation describing the dynamics of the density operator for atoms in the lattice. In what follows, we set $\gamma_{0000} \equiv \gamma$, so that in the Lamb-Dicke limit $\eta \ll 1$, $\gamma_{1010} = \gamma_{0101} = \eta^2\gamma$. We also use the symbols $U \equiv U^{(0,0,0,0)}$ and $J = J(0)$.

Physical interpretation of the master equation – The key effect of spontaneous emissions is that the environment (in this case the external electromagnetic field) measures the position of an atom, effectively localizing the atom undergoing a spontaneous emission event on a length scale given by the wavelength of the scattered photon. Since the wavelength is comparable to the lattice spacing $\lambda \sim a$, this quantitatively corresponds to localization of the atom on a single lattice site as depicted in Fig. 1a. Assuming we do not measure the photon field, an initially delocalized state of a single atom, e.g., an eigenstate of quasimomentum \mathbf{q} on the lattice $|\mathbf{q} = 0\rangle \propto \sum_{\mathbf{i}} b_{\mathbf{i}}^{(0)\dagger} |\text{vac}\rangle$ is decohered into a mixture of

different possible atom locations. If the atom remains in the lowest Bloch band, then $\rho = |\mathbf{q} = 0\rangle\langle\mathbf{q} = 0| \rightarrow \sum_{\mathbf{i}} b_{\mathbf{i}}^{(0)\dagger} |\text{vac}\rangle\langle\text{vac}| b_{\mathbf{i}}^{(0)}$, and the atom is spread over the entire Brillouin zone in quasi-momentum space.

Overview of thermalization – As energy is added to the system via the dissipative process, it is often postulated that Hamiltonian dynamics should be able to thermalize the added energy, in the sense that simple observables attain values corresponding to a thermal distribution with the new mean energy value $\langle E \rangle$. However, the case of inter-band excitations is a clear counterexample, as the added energy is of the order of band-gap energy $\omega_g = \omega^{(1)} - \omega^{(0)}$, and cannot be thermalized on experimental timescales due to a mismatch with the energy scales of the lowest Bloch band $\omega \gg U, J$. [40]. This is analogous to the collisional stability of doublon pairs demonstrated in recent experiments [31].

For intra-band processes, it might be expected that the system will thermalize, due to the non-integrability of the Bose-Hubbard model except for very small or large values of U , similar to what is expected for a quantum quench of U/J [32]. However, it is not clear that this readily applies to our situation because a spontaneous emission event leads to localization of atoms in a *local quantum quench* with excitations that are very low in energy. This may result in a lack of thermalization for all values of U given the integrable nature of the spectrum at low energies. Below we find that the relaxation timescales and equilibrium values strongly depend on the interaction characteristics in the lower band.

Thermalization after a single intra-band spontaneous emission event – In order to characterize the thermalization process, we first consider the situation where the system is in the ground state of the single-band Bose-Hubbard model $|\psi_g\rangle$ at time $t = 0$, and then undergoes a spontaneous emission occurring at site \mathbf{i} . In the sense of continuous measurement theory [19], the state prepared in this way is

$$|\psi_i(t = 0^+)\rangle = \frac{b_{\mathbf{i}}^{(0)\dagger} b_{\mathbf{i}}^{(0)} |\psi_g\rangle}{\|b_{\mathbf{i}}^{(0)\dagger} b_{\mathbf{i}}^{(0)} |\psi_g\rangle\|}. \quad (4)$$

We consider a weighted ensemble average over the sites \mathbf{i} with probabilities of spontaneous emission $p_i \propto \langle \psi_g | n_{\mathbf{i}}^2 | \psi_g \rangle$, and treat a 1D system, where we can use t-DMRG methods to propagate the state exactly in time. However, we expect the mechanisms for thermalization that we discuss to also apply in higher dimensions. Note that these DMRG results are converged in the matrix product state bond dimension D and the truncation of the local dimension, d_l .

Fig. 1b shows the typical dynamics after a spontaneous emission spreads a particle over the whole Brillouin zone and increases the kinetic energy E^{kin} . The interactions between particles transfer some of this increased kinetic energy to interaction energy, as shown

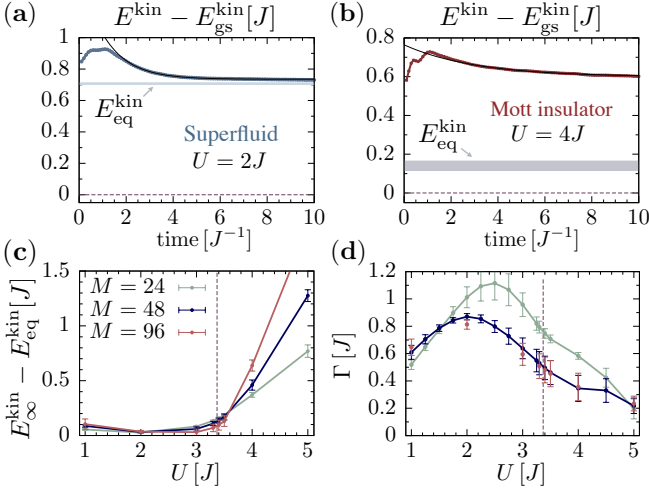


FIG. 2: (Color online) Time evolution of the kinetic energy after a single spontaneous emission event (averaged over jumps on all possible sites). (a - b) For a superfluid initial state ($U = 2J$), the kinetic energy relaxes to the equilibrium value obtained from a Monte-Carlo calculation $E_{\text{eq}}^{\text{kin}}$. For MI states ($U = 4J$), the energy relaxes, but not to $E_{\text{eq}}^{\text{kin}}$. The zero value of kinetic energy for this plot is the ground state kinetic energy $E_{\text{gs}}^{\text{kin}}$. (c) The difference of the infinite time value of the kinetic energy (obtained from an extrapolation of an exponential fit) to the Monte-Carlo equilibrium energy. For MI states with $U/J \gtrsim 3.37$, the difference increases rapidly for system sizes $M = 24, 48, 96$ sites (d) The decay rate extracted from the exponential fit as a function of U . (t-DMRG results, $d_t = 6$, $D = 256, 512$; error bars represent fitting errors and statistical errors from QMC).

explicitly in Fig. 2a for an initial superfluid (SF) state with $U = 2J$. At $t = 0^+$, E^{kin} is increased by of the order of J over the ground state value, and it then relaxes to lower value over a timescale $\sim 5/J$ in unitary time evolution. We obtain an equilibrium value $E_{\text{eq}}^{\text{kin}}$ from path integral Monte-Carlo (QMC) calculations with worm-type updates [33] (here in the implementation of Ref. [34] – see Ref. [35] for a recent review of the method with applications to cold gases) at finite temperature T , fitting T to match the value of energy $\langle E \rangle$ for $t \geq 0^+$. It is remarkable that this value corresponds to the equilibrium value reached dynamically within statistical errors, indicating thermalization of this quantity. In contrast, for an initial Mott Insulator (MI, $U = 4J$) state, E^{kin} relaxes on an only slightly longer timescale to an equilibrium value that clearly does not correspond to a thermal distribution at the appropriate value of $\langle E \rangle$. In fact, in this parameter regime, thermally induced coherence in the MI leads to a $E_{\text{eq}}^{\text{kin}}$ being close or even below the value of the ground state kinetic energy [36].

In Fig. 2c we compare the extrapolated equilibrium kinetic energy, E_{∞}^{kin} (obtained from an exponential fit) to $E_{\text{eq}}^{\text{kin}}$ for various system sizes and interaction strengths. In the SF regime 1D Bose-Hubbard model we observe re-

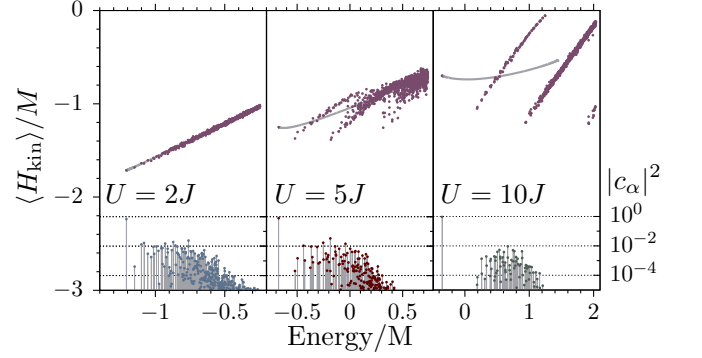


FIG. 3: (Color online) Expectation values of the kinetic energy of the lowest 1000 eigenstates as a function of the energy E in a system with $M = 10$ sites and $N = 10$ particles (exact diagonalization). The grey line in the upper plot shows the distribution of the energy for a canonical ensemble with temperature T fitted to give mean energy E . In the SF, the eigenvalue expectations are distributed around the Boltzmann distribution, but are far from these values in the MI. The lower parts show the corresponding occupation probabilities for eigenstates after a single spontaneous emission.

laxation of E_{∞}^{kin} to $E_{\text{eq}}^{\text{kin}}$, while in the MI regime it is far from the thermal value. While we might expect for very large values of U that thermalization would become difficult as the Bose-Hubbard model approaches an integrable system with hard-core bosons [10, 37], the lack of thermalization for values of U/J immediately above the SF-MI transition point (when the gap is about $\Delta = J/8$) is very striking [41]. Before performing these calculations, we might have expected a crossover behavior, similar to that seen in the relaxation rates, as shown in Fig. 2d from exponential fits to the long-time behavior of E^{kin} .

The key to understanding this behavior lies in the fact that the spontaneous emissions give rise to a local quantum quench, which only significantly populates low-energy eigenstates of the Hamiltonian. Most of the amplitude of the resulting wavefunction is in the ground state, as shown in Fig. 3, where we plot occupation probabilities $|c_{\alpha}|^2$ and expectation values of the kinetic energy $\langle E_{\alpha} | \hat{E}^{\text{kin}} | E_{\alpha} \rangle$ in the lowest 1000 energy eigenstates $|E_{\alpha}\rangle$. We see that E^{kin} grows essentially linearly as a function of E_{α} , even for $U/J \sim 3$ near the phase transition, and that these values coincide with $E_{\text{eq}}^{\text{kin}}$ from a Boltzmann distribution. Because of the approximate linear dependence, averages over states with different $|c_{\alpha}|^2$ distributions will still be approximately equal. Thus, the long time average $\langle E^{\text{kin}} \rangle \rightarrow \sum_{\alpha} |c_{\alpha}|^2 \langle E_{\alpha} | \hat{E}^{\text{kin}} | E_{\alpha} \rangle$ [5] will correspond to the value for the Boltzmann distribution. As soon as we enter the MI phase, between $U/J \approx 3$ and $U/J \approx 3.8$, there is a qualitative change in the distribution of $\langle E_{\alpha} | \hat{E}^{\text{kin}} | E_{\alpha} \rangle$ values, as depicted in Fig. 3, after which we cannot expect to obtain thermal values. In the deep MI, the $\langle E_{\alpha} | \hat{E}^{\text{kin}} | E_{\alpha} \rangle$ values are far from $E_{\text{eq}}^{\text{kin}}$, and

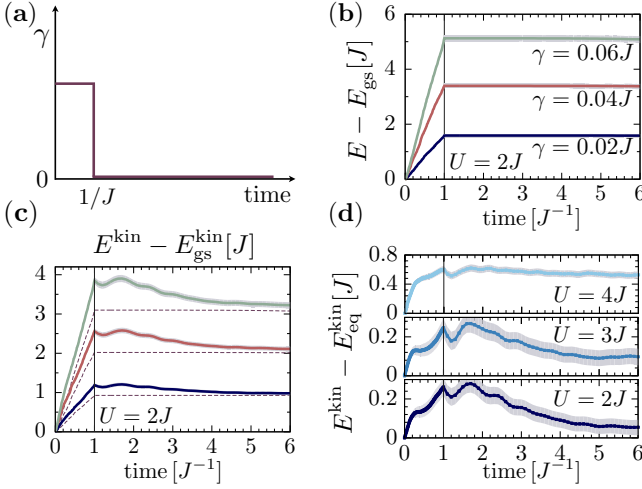


FIG. 4: (Color online) Quantum trajectory simulation for heating which is switched on for a time $t = 1/J$, as illustrated in (a). Heating rates are rates $\gamma = 0.02J, 0.04J, 0.06J$. Results are for system of 48 atoms on 48 sites, the standard error of the mean is given as shaded area. (b) The increase of the total energy during the heating process for a superfluid state ($U = 2J$). (c) The increase in kinetic energy during the heating and the subsequent relaxation. For superfluid initial states, the kinetic energy relaxes to the equilibrium value (QMC calculations, dashed lines). For a Mott insulating initial state, on the same time-scale, the energy does not thermalize. This can be seen in (d) where we plot the difference between the actual kinetic energy and the equilibrium energy (t-DMRG results, $D = 256$, $d_l = 6$, 500 trajectories).

correspond to excitation of doublon-holon pairs.

Note that as with thermalization in any closed quantum system, the behavior depends on the observable considered, and sufficiently complicated or non-local observables will never thermalize [5]. When we consider the quasi-momentum distribution n_q in our system with open boundary conditions, we find that for large $q \gtrsim 1/(2a)$, values agree well with a thermal distribution on timescales $tJ \sim 5$ in the SF for $U \gtrsim 1$. However, long wavelength modes around $n_{q=0}$ require much longer relaxation timescales. In the MI, the distribution behaves qualitatively differently, in that all values of q show small discrepancies from the equivalent thermal values, consistent with what we observed for the kinetic energy.

Finite-time light scattering and comparison with thermal distributions – We now consider a specific experimental setup in which these effects could be observed. As depicted in Fig. 4a, we consider a situation in which the background scattering rate is low, and then a moderate scattering rate is induced for a short time $t = 1/J$ (e.g., via a weak beam with near-resonant light). We then switch this off, and observe how the system thermalizes over a timescale of $t \sim 5/J$. We compute the dynamics of this process by combining t-DMRG methods with quantum trajectory techniques, which after a

stochastic average allow us to determine the many-body dynamics from the master equation.

As shown in Fig. 4b, the total energy of the system will increase when $\gamma \neq 0$, but will remain constant once the dissipation is removed. If we denote the kinetic energy term of the Hamiltonian for band (\mathbf{n}) by $H_J^{(\mathbf{n})} = -\sum_{\mathbf{n}, \langle i, j \rangle} J^{(\mathbf{n})} b_i^{(\mathbf{n})\dagger} b_j^{(\mathbf{n})}$, then the time-dependence of the total energy from intra-band processes in the lowest Bloch band is given by

$$\frac{d}{dt}\langle E \rangle = \frac{d}{dt}\langle H \rangle = -\gamma\langle H_J^{(0)} \rangle = -\gamma\langle E^{\text{kin}} \rangle. \quad (5)$$

Because the lowest Bloch band for a single particle has energies in the range $[-2J^{(0)}, +2J^{(0)}]$, the E^{kin} will typically be large and negative in the many-body ground state, so that this corresponds to a strong increase in the energy of the system, as observed in Fig. 4b.

Correspondingly, the kinetic energy will increase. In Fig. 4c, we plot E^{kin} and $E_{\text{eq}}^{\text{kin}}$ as a function of time. As expected from the arguments above, the kinetic energy increases much faster than would be expected from a thermal distribution with the same increase in total energy, and how far away the values are from a thermal distribution is dependent on γ . Note that in the experiment of Ref. [24], $\gamma \approx 0.02J$. In Fig. 4d we plot $E^{\text{kin}} - E_{\text{eq}}^{\text{kin}}$ for different values of U/J . We see clearly that as in the case of a single spontaneous emission event above, the kinetic energy will relax towards the expected equilibrium values in the superfluid regime. Strikingly, this is not the case in the Mott Insulator, where the system remains well away from the equilibrium value on the timescales calculated. Note that while here the energy increase is small, as we use parameters where few spontaneous emission events occur to allow quantitative numerical treatments, experiments could work with larger increases through faster scattering rates or longer excitation timescales.

Conclusions – We showed that for bosons in an optical lattice, a qualitative change in the thermalization behavior after spontaneous emission events will occur at the SF-MI transition point. Certain simple quantities including the kinetic energy and quasi-momentum distribution settle rapidly to a steady state. However, while in some cases these values correspond to a thermal distribution, in others the values are demonstrably non-thermal. These findings, presented here for a uniform system, remain valid in the presence of a harmonic trap, as is shown by results presented in the supplementary material. The lack of complete thermalization implies that the specific effects on specific many-body states must be considered.

For the realization of low-temperature states in optical lattices, this may lead in some regimes to a greater robustness of the states being produced, as thermalization of all the energy added in a spontaneous emission event would often lead to temperatures above those required for realization of fragile types of order [22–25]. Instead, because the dynamics must be treated as a non-equilibrium

situation on a case-by-case basis, much of the interesting order in the state can survive on substantial timescales.

We thank I. Bloch, D. Boyanovsky, W. Ketterle, S. Langer, H. Pichler, U. Schneider, D. Weiss, and P. Zoller for helpful and motivating discussions. This work was supported in part by AFOSR grant FA9550-12-1-0057, and by a grant from the US Army Research Office with funding from the DARPA OLE program. Computational resources were provided by the Center for Simulation and Modeling at the University of Pittsburgh.

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 - [40] Note that collisional processes between two or more atoms in the first excited band can return particles to the lowest band while exciting atoms to higher bands. This doesn't affect the conclusion that the bandgap energy cannot be thermalized with the atoms in the lowest band.
 - [41] Although from our calculations we cannot rule out a second relaxation process to a thermal distribution for much larger systems or on much longer timescales, it is clear that a striking qualitative change in behavior occurs here, leading to a lack of thermalization on typical experimental timescales

SUPPLEMENTAL MATERIAL

EXCITATIONS TO HIGHER BANDS

The intra-band processes described in the main text will dominate the dynamics for red-detuned optical lattices, and spontaneous emissions induced by near-resonant light with a constant intensity profile. This dominance could be increased by adding an additional step in which the lattice is made very deep, and the interactions very weak during the process of scattering near-resonance light. This decreases η^2 , and thus the probability of inter-band processes. Band-mapping techniques are also an important diagnostic tool to determine the occupation of higher bands [38].

Here we consider also the case of a spontaneous emission event, which takes an atom to the first excited band and study the time evolution of the state

$$|\psi_i(t=0^+)\rangle = \frac{b_i^{(1)\dagger} b_i^{(0)} |\psi_g\rangle}{||b_i^{(1)\dagger} b_i^{(0)} |\psi_g\rangle||} \quad (6)$$

under the two-band Bose-Hubbard model, *i.e.*, the Hamiltonian $H = H_0 + H_1 + H_{01}$, where $H_{0,1}$ is the respective single band Bose-Hubbard Hamiltonian for each band, and $H_{01} = (U_{01}/2) \sum_i b_i^{(1)\dagger} b_i^{(1)} b_i^{(0)\dagger} b_i^{(0)}$ with $U_{01} = U^{1,0,1,0}$. Since we consider a transition to the first excited band, the tunneling amplitude in this band $J^{(1)} < 0$, and we consider a shallow lattice with $V_0 = 5E_R$, so that $J^{(1)} \approx -7J$. Furthermore, typically $U_{01} \approx U$ and we choose the two to be equal. After the spontaneous emission $\langle H_1 \rangle = 0$, since the particle in the excited band is localized and there is no interaction. As shown in Fig. 5a, we see that in the subsequent evolution the particle in the excited band starts to delocalize, thereby lowering its energy. Through collisions with particles in the lowest band, energy is transferred to the lowest band and $\langle H_0 \rangle$ increases. On the timescale of our simulation no steady state is achieved.

EFFECTS OF A HARMONIC TRAP

In a realistic experimental setup, the particles will always be confined by a harmonic trap. This can lead to situations, in which parts of the system have superfluid components despite the fact that $U/J > 3.37$. In Fig. 5b we show results for the evolution after a single spontaneous emission events, *i.e.*, of the state (4) in the presence of a harmonic confinement $\varepsilon_i = \omega_T \sum_i (i - i_0)^2$ (center site $i_0 = (M+1)/2$) with $\omega_T = 0.012J$ for a system with $M = 48$ sites. We again average over jumps on all possible sites weighted with the probabilities $p_i \propto \langle \psi_g | n_i^2 | \psi_g \rangle$. In the upper panel we find thermalization for the kinetic energy in the superfluid state with $U = 2J$. As in the case of box boundary conditions, the kinetic energy relaxes to a value corresponding to a thermal distribution on the experimentally relevant time-scales. For larger interactions ($U = 5J$), we see from the density profile (insets) that the system is not in a MI state with unit filling (these appear only for values around $U/J \sim 10$). Nevertheless, in this case we find that the system does not relax to a value of a thermal distribution. Note that the Monte-carlo thermal kinetic energy in this case is in fact above the value after the jump. In the case of a Mott insulator in a trap ($U = 10J$) with unit filling (seen by the density profile in the inset), we find that the system does not approach a steady state kinetic energy but shows oscillations, which can be explained by boundary effects of deflected doublon-hole pairs (see below).

DOUBLON HOLON RESULTS FOR STRONG INTERACTIONS

In the limit of strong interactions we can show that there cannot be any thermalization even far away from the regime where the system assumes an ideal or a hard-core boson Mott-insulator [10, 37]. Therefore we perform calculations in a regime where we can restrict the occupations of each site to 0, 1, and 2 bosons. In this regime one can map the system to a model of free fermionic doublon-holon pairs. Using a generalized Jordan-Wigner transformation as described in [39], it is straightforward to show that the time-evolved state after the spontaneous emission on site m is

$$\begin{aligned} |\psi(t)\rangle &\propto |\text{vac}\rangle + \frac{1}{M} \sum_{q,q'} e^{ima(q-q')} w(q, q') \\ &\times e^{-it[\epsilon_d(q') - \epsilon_h(q)]} c_{d,q'}^\dagger c_{h,-q}^\dagger |\text{vac}\rangle. \end{aligned} \quad (7)$$

Here, the state $|\text{vac}\rangle$ is the vacuum, which is annihilated by the free quasi-particles c_d and c_h , which are superpositions of double occupied sites and holes. $w(q, q')$ is a characteristic wave-packet (example shown in Fig.5c), and the

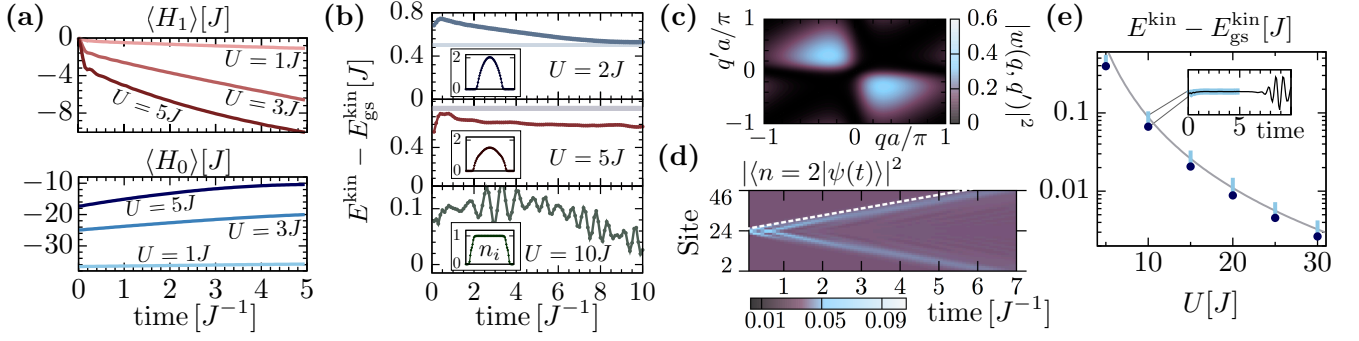


FIG. 5: (Color online) (a) Time evolution of the energy in the two lowest bands after a single spontaneous emission, which takes a particle to the excited band (averaged over all sites) ($M = N = 24$, t-DMRG results, $D = 256$, $d_l^{[1]} = 6$, $d_l^{[2]} = 2$) (b) Relaxation in the lowest band in the presence of a harmonic trap ($\omega_T^2 = 0.012J$, $N = 48$, $M = 64$). The insets show the initial density profiles of the ground-states in the trap. (t-DMRG results, $D = 512$, $d_l = 6, 8$) (c) The doublon-holon wave packet created by a single spontaneous emission in the center of the system for $U = 10J$. (d) Time-dependent double occupancy, which reveals the propagation of the wave-packet (dashed white line: analytical result) (e) Results for the time-evolution of the kinetic energy for strong interactions. The inset shows the evolution after the spontaneous emission. Boundary effects become important once the wave-packet reaches the boundary. The kinetic energy is nearly constant as function of time and matches the analytical result (grey line) (t-DMRG results, $D = 512$, $d_l = 6$).

dispersion relations for $c_{d/h}$ are denoted by $\epsilon_{d,h}(q)$. As shown in Fig. 5d, after a spontaneous emission the free particles spread through the system with a characteristic group velocity before boundary effects become important.

In addition, from state (7) it is straightforward to show, that any observable in quasi-momentum space, *i.e.*, any operator, which can be written in the form $\hat{O} \equiv \sum_q \hat{O}_q$ such as the kinetic energy is time-independent, and therefore no relaxation is possible in this regime. In Fig. 5e we compare the analytical result for the difference of the kinetic energy to the ground-state to a numerical t-DMRG simulation after a single spontaneous emission in the center of the system. We find that in agreement to the doublon-holon calculation, the kinetic energy after the jump remains nearly constant (up to some small initial increase due to higher order effects) as long as boundary effects become important at $tJ \sim 6$.